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LETTER TO THE EDITOR

Probable detection of H_2D^+ in the starless core Barnard 68

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ABSTRACT

Context. The presence of H_2D^+ in dense cloud cores underlies ion-molecule reactions that strongly enhance the deuterium fractionation of many molecular species.

Aims. We determine the H_2D^+ abundance in one starless core, Barnard 68, that has a particularly well established physical, chemical, and dynamical structure.

Methods. We observed the ortho- H_2D^+ ground-state line $1_{10-1_{11}}$, the N_2H^+ $J = 4-3$ line, and the H^{13}CO^+ $4-3$ line with the APEX telescope.

Results. We report the probable detection of the o- H_2D^+ line at an intensity $T_{\text{mb}} = 0.22 \pm 0.08$ K and exclusively thermal line width, and find only upper limits to the N_2H^+ $4-3$ and H^{13}CO^+ $4-3$ intensities.

Conclusions. Within the uncertainties in the chemical reaction rates and the collisional excitation rates, chemical model calculations and excitation simulations reproduce the observed intensities and that of o- H_2D^+ in particular.

Key words. ISM: abundances – ISM: individual objects: Barnard 68 – ISM: molecules – submillimeter

1. Introduction

The densest and coldest cores of interstellar molecular clouds are receiving much attention as the possible precursors of star formation. Often referred to as starless or pre-protostellar cores, they are characterized chemically by a large depletion of molecules as they freeze out onto dust grains, and an associated increase in the relative abundance of deuterated isotopomers of numerous species (e.g., Kuiper et al. 1996; Ceccarelli et al. 1998; Loinard et al. 2002; Bacmann et al. 2003; Caselli et al. 2003; Stark et al. 2004). This increase is explained by the reaction $\text{H}_3^+ + \text{HD} \rightleftharpoons \text{H}_2\text{D}^+ + \text{H}_2$, which is favored in the forward direction at low temperatures, and subsequent ion-molecule reactions involving H_2D^+ . Detection of H_2D^+ in dense cloud cores directly tests this proposed mechanism. Through its spectral line shape it also probes the core's velocity field, in regions where all other molecular tracers are strongly depleted. First predicted by Dalgarno et al. (1973), the ground-state transition of ortho- H_2D^+ , $1_{10-1_{11}}$, lies in the submillimeter wavelength range near 372 GHz, in a region with poor atmospheric transmission. Under excellent observing conditions on Mauna Kea (Hawai'i), H_2D^+ has been successfully detected toward astronomical sources, including the young stellar object NGC 1333 IRAS 4A (Stark et al. 1999), the starless core L1544 (Caselli et al. 2003), and the circumstellar disks of TW Hya and DM Tau (Ceccarelli et al. 2004; but also see Guilloteau et al. 2006).

This Letter reports the probable detection of the H_2D^+ $1_{10-1_{11}}$ line toward the well-studied starless core Barnard 68 conducted with the Atacama Pathfinder EXperiment (APEX¹) telescope on Chajnantor (Chile).

Barnard 68 (B68) is one of the most extensively studied starless cores. Using stellar extinction measurements, its density structure has been found to be well matched by a near-critical Bonnor-Ebert sphere (Alves et al. 2001). Bonnor-Ebert spheres (Ebert 1957; Bonnor 1958) describe the equilibrium configuration of self-gravitating cloud cores just before the onset of collapse. Bergin et al. (2002) found strong depletion of C^{18}O in B68. Lada et al. (2003) analyzed the velocity field of B68, and found that the line widths in the center are close to thermal, leaving no room for significant turbulent motion. In the outskirts of the core, line centroid shifts suggest a non-radial pulsating motion.

With the successful commissioning of APEX, the 372 GHz ground-state transition of ortho- H_2D^+ has come within reach of regular observing, given the good local weather conditions. This Letter presents the probable detection of H_2D^+ toward the center of this starless core obtained during the Science Verification

¹ This publication is based on data acquired with the Atacama Pathfinder EXperiment (APEX). APEX is a collaboration of the Max-Planck-Institut für Radioastronomie, the European Southern Observatory, and the Onsala Space Observatory.

of APEX (Sect. 2) and discusses the emission strength in the framework of a chemical model including depletion and deuteration (Sect. 3).

2. Observations and results

The APEX telescope observed the H_2D^+ $1_{10}-1_{11}$ line at 372.421385 GHz on 2005 July 24 and 25 using the APEX-2a receiver and the FFTS backend with a bandwidth of 1 GHz and 16384 channels. This frequency setting also covers the N_2H^+ $J = 4-3$ line at 372.6725090 GHz. The telescope was pointed at the A_V peak measured by Alves et al. (2001) at $\alpha_{2000} = 17^{\text{h}}22^{\text{m}}38^{\text{s}}.6$ and $\delta_{2000} = -23^{\circ}49'46''.0$. The observations were taken in position-switched mode, using an emission-free reference position. Pointing was checked on the nearby object RAFGL 1922. During the observations the source was at elevations of $25^{\circ} - 40^{\circ}$. A precipitable water vapor column of 0.47 mm resulted in DSB system temperatures of 150–250 K. On 2005 July 25, the H^{13}CO^+ $J = 4-3$ line at 346.998546 GHz was observed with a similar set up. After the observations, the velocity scale of the spectra was recalculated by the telescope staff to correct for a small (0.1 km s^{-1}) inaccuracy during data taking.

After careful inspection of the data, the individual 30 sec scans were averaged using the CLASS software package; a total integration time (on+off) of 36 min was obtained for the H_2D^+ line (12.6 min for H^{13}CO^+). A sinusoidal baseline with a period of $\sim 350 \text{ km s}^{-1}$ was removed, followed by a first order baseline in the area surrounding the expected line. After smoothing the spectral resolution to 0.098 km s^{-1} , a rms noise level of 0.059 K on the T_A^* scale was found (0.058 K for H^{13}CO^+ in 0.11 km s^{-1} channels), adopting a forward efficiency of 0.97. The data were subsequently transformed to the main beam antenna temperature scale by division by 0.73, the recommended mean beam efficiency in the 345 GHz band (Güsten et al. 2006).

The H_2D^+ line was detected at a signal-to-noise ratio of ~ 3 (Fig. 1). Fitting a single Gaussian line to the spectrum yields $T_{\text{mb}} = 0.222 \pm 0.082 \text{ K}$, $V_{\text{LSR}} = 3.36 \pm 0.05 \text{ km s}^{-1}$, $\Delta V = 0.33 \pm 0.1 \text{ km s}^{-1}$, and an integrated line intensity of $0.078 \pm 0.015 \text{ K km s}^{-1}$. Although the line peak is detected at only 2.7σ , the integrated intensity is detected at 5.2σ , and we argue that the detection of H_2D^+ in B68 is probable (only deeper integration can make the result more secure). Figure 3 shows the H_2D^+ spectrum over a 200 km s^{-1} range. Out of the 1018 channels in this part of the spectrum, only 4 exceed the 3σ level (0.4%), as statistically expected. The significance of the detection is further supported by the close match to the source V_{LSR} of $3.36-3.37 \text{ km s}^{-1}$ and the purely thermal line width of 0.33 km s^{-1} (H_2D^+ at 10 K), as found by Lada et al. (2003) for N_2H^+ and C^{18}O . All other peaks are much narrower (1–2 channels). Because H_2D^+ retains a high abundance at the center of the core (see below), the apparent absence of turbulent motion in the H_2D^+ line provides strong support for the conclusion of Lada et al. (2003) that B68 is exclusively thermally supported. This situation is very different from the velocity field in, e.g., L1544, which shows significant velocity gradients and wider H_2D^+ lines (van der Tak et al. 2005). No detection was made of either the N_2H^+ $4-3$ line to a 2σ upper limit of 0.16 K or the H^{13}CO^+ $4-3$ line to 2σ of 0.18 K. An emission peak at the correct V_{LSR} for the N_2H^+ transition and the expected thermal width of 0.075 km s^{-1} is likely noise.

In the documents accompanying the data release, it was noted that lines tuned in the upper sideband of APEX-2a could be too strong by 40%. This effect has been shown to be present

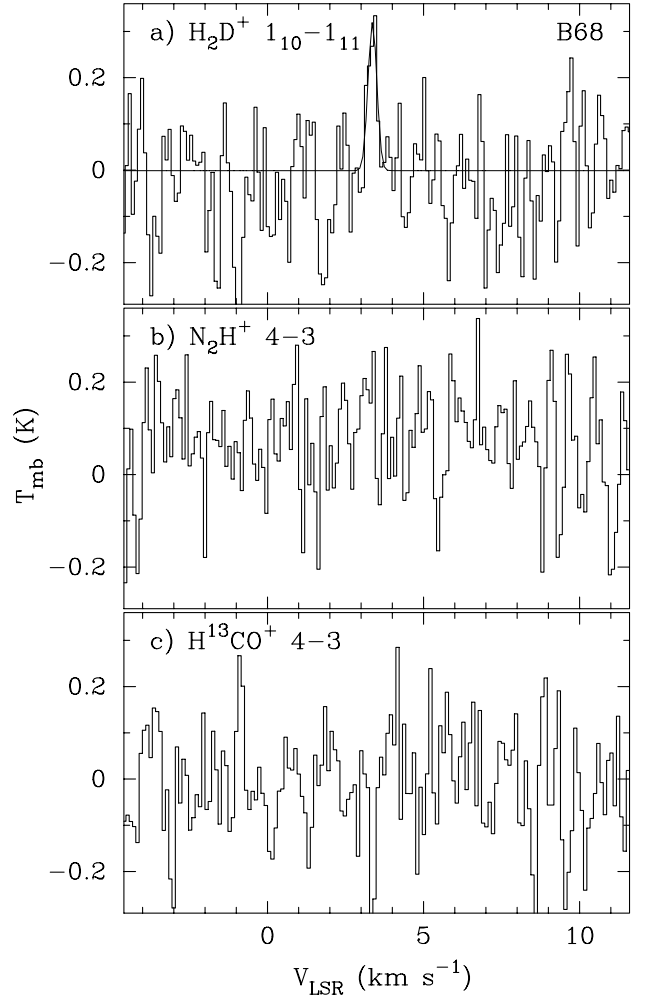


Fig. 1. **a)** Detection spectrum of H_2D^+ $1_{10}-1_{11}$ toward the center of B68 (histogram), with the best-fit Gaussian line profile superposed (thin line). The model of Sect. 3 yields an identical profile for the modified collisional excitation rates as discussed. **b)** Non-detection of N_2H^+ $4-3$ at the same position. **c)** Non-detection of H^{13}CO^+ $4-3$ at the same position.

for ^{12}CO $J = 3-2$, and is thought to be due to a resonance near the CO line frequency. It is therefore unlikely that our H_2D^+ observations suffer from this effect, although no sideband-ratio measurements are available to confirm this.

3. Discussion

At the detected line strength of $0.22 \pm 0.08 \text{ K}$, the H_2D^+ line is weaker than detections toward other starless cores such as L1544 ($\sim 1 \text{ K}$). Two aspects distinguish B68 from L1544. First, B68's H_2 column density is lower than that of L1544, at $3.6 \times 10^{22} \text{ cm}^{-2}$ and $(6-13) \times 10^{22} \text{ cm}^{-2}$ (Alves et al. 2001; Ward-Thompson et al. 2002, 1999). Secondly, B68's central density of $2 \times 10^5 \text{ cm}^{-3}$ is lower by a factor of 6 than that of L1544. Given that the critical density of the ground-state transition of ortho- H_2D^+ is $\sim 2 \times 10^6 \text{ cm}^{-3}$ (for our adopted collision rate; see below), a careful analysis is required to test whether the decreased line strength is due to (a combination of) sub-thermal excitation, lower total column density, or lower abundance of this key deuterated species.

From the strength of the H_2D^+ line, assuming optically thin conditions, we derive a beam-averaged column density of

$N(\text{H}_2\text{D}^+) = (1.5 \pm 0.14) \times 10^{12} \text{ cm}^{-2}$ for an excitation temperature of 10 K. This corresponds to thermal equilibrium excitation at the kinetic temperature in B68. Given the critical density quoted above, it is highly likely that the excitation is subthermal, requiring a larger column density to reproduce the emission. For example, an excitation temperature of 5 K implies $N(\text{H}_2\text{D}^+) = (1.0 \pm 0.3) \times 10^{13} \text{ cm}^{-2}$. This column density corresponds to an average H_2D^+ abundance with respect to H_2 of $(2.9 \pm 0.9) \times 10^{-10}$.

Further insight in the H_2D^+ abundance can be obtained from modeling the chemistry in the B68 core followed by a statistical equilibrium calculation of the H_2D^+ excitation and line radiative transfer. Following Vastel et al. (2006) we use the simple chemical model of Caselli et al. (2002), updated to include the multiply deuterated forms of H_3^+ and the new values of the binding energies of CO and N_2 (Öberg et al. 2005). B68 is modeled as a spherical cloud with radius 12 000 AU and the density profile fitted to the Bonnor-Ebert solution by Tafalla et al. (2002, 2004). The temperature profile follows that of L1544 (Young et al. 2004), resulting in a temperature gradient from 13 K at the core edge to 9.8 K at its center.

The chemical model starts with fully undepleted abundances of CO, N_2 , and O, and lets the species interact with and freeze-out on the dust grains which follow a MRN size distribution (Mathis et al. 1977) with a minimum grain size of $0.005 \mu\text{m}$. Assuming that the ion chemistry is fast compared to depletion, the molecular ions follow from the instantaneous neutral abundances. Following Vastel et al. (2006) a cosmic-ray ionization rate of $1.3 \times 10^{-17} \text{ s}^{-1}$ and sticking coefficient to $S = 1.0$ (Burke & Hollenbach 1983) are adopted. Finally, for H_2D^+ an ortho-to-para ratio of 1.0 is adopted as expected at low temperatures (Gerlich et al. 2002). We note that the results of these calculations may depend quite sensitively on the chemical reaction rates and their dependence on temperature (Emprechtinger et al. in preparation), including the H_2D^+ destruction reaction with H_2 (Schlemmer et al. 2005 and Asvany et al., in preparation).

Figure 2 shows the resulting abundance profiles of some relevant species. Typical H_2D^+ abundances with respect to H_2 at the center of B68 are predicted to be 4×10^{-10} . The corresponding H_2D^+ column density is $5.0 \times 10^{12} \text{ cm}^{-2}$, close to the beam-averaged column density of $1 \times 10^{13} \text{ cm}^{-2}$ found from the simple analysis above.

With these abundance profiles, the statistical equilibrium excitation is calculated using the code of Hogerheijde & van der Tak (2000). The velocity field is assumed to be static with only thermal broadening and no turbulent motion. We ignore the significant motion in the outer regions of the core reported by Lada et al. (2003), since our observations are taken to the core's center and the observed spectrum shows no indication of line broadening. The resulting spectrum is convolved in a $17''$ FWHM beam appropriate for APEX at these wavelengths, yielding intensities on the T_{mb} scale; a distance of 100 pc is adopted for B68.

These calculations require reliable collisional rate coefficients, which are not available in the literature. We follow van der Tak et al. (2005) in adopting estimated rates, and investigate the effect of their inherent uncertainty. Using these rates, we find a $\text{H}_2\text{D}^+ 1_{10}-1_{11}$ intensity of 0.10 K, lower by a factor of 2 than observed. Increasing the collisional rates by a factor of three, entirely within the estimated uncertainty, increases the emergent intensity to 0.24 K. Varying the rates by factors of 10 up or down produces a range of intensities of 0.011–0.48 K. The opacity of the line is 0.13 and the excitation temperature

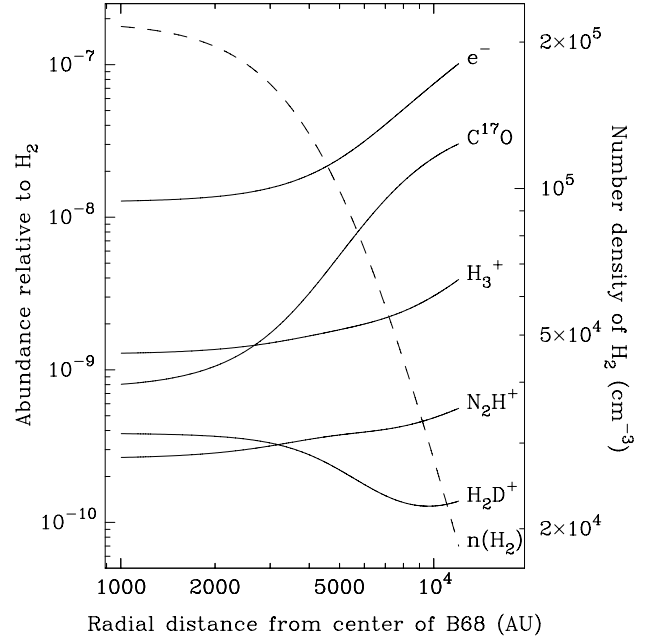


Fig. 2. Predicted abundances of several key species in the H_2D^+ modeling (solid lines) and H_2 number density (dashed line) as functions of radius in B68.

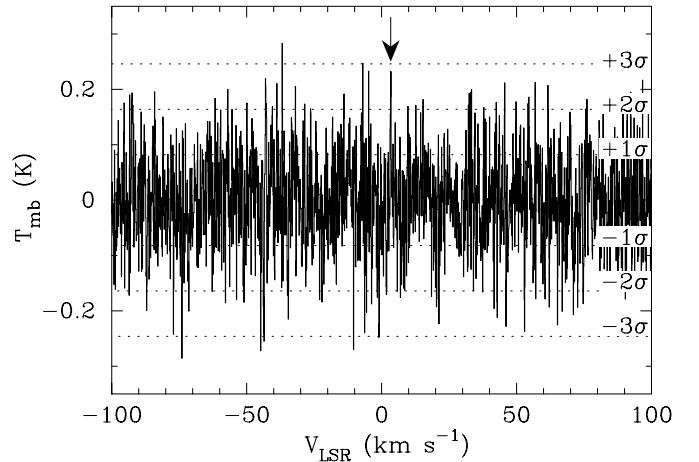


Fig. 3. Detection spectrum of $\text{H}_2\text{D}^+ 1_{10}-1_{11}$ toward the center of B68 over a baseline range of 200 km s^{-1} . Noise levels at $\pm 1\sigma$, $\pm 2\sigma$, and $\pm 3\sigma$ are indicated. The arrow indicates the V_{LSR} of B68 of 3.36 km s^{-1} .

ranges from 3 to 6 K, consistent with the simple assumptions made above.

We conclude that the observed intensity of H_2D^+ is consistent with chemical model predictions, but that the uncertainty in the available collisional rate coefficients precludes a detailed comparison, especially for subthermal excitation. Determination of more reliable rates is clearly warranted. van der Tak et al. (2005) reach the same conclusion, including a preference for collision rates enhanced by factors 3–10; like these authors, we refrain from recommending adjusting the collision rates because of the uncertainties in the chemical modeling.

Using collisional rates from the Leiden data base (Schöier et al. 2005), our model calculations are compatible with the upper limits on H^{13}CO^+ and $\text{N}_2\text{H}^+ 4-3$ reported here, as well the N_2H^+ and $\text{C}^{18}\text{O} 1-0$ detections of Bergin et al. (2002) and $\text{N}_2\text{H}^+ 3-2$ from Crapsi et al. (2005). Quantitatively, we find

19 mK for H^{13}CO^+ 4–3 (observed: <0.15 K, 2σ); 0.79 K km s^{-1} for C^{18}O 1–0 (0.85 K km s^{-1}). Our model overproduces the N_2H^+ emission by about a factor of 2; we find 0.38 K for N_2H^+ 4–3 (observed <0.16 K, 2σ), and values of 3.8 K km s^{-1} for N_2H^+ 1–0 (observed, 2.5 K km s^{-1}) and 0.35 K km s^{-1} for 3–2 (observed, 0.17 K km s^{-1}).

We conclude that our detection of H_2D^+ toward B68 is consistent with models for the deuterium chemistry in starless cores which also reproduces other observed lines. However, the lack of reliable collision rates precludes any stronger statements about the H_2D^+ chemistry. Given the pivotal role of H_2D^+ in deuterium chemistry and the well studied nature of B68, calculation of such rates is warranted, especially now that observations of H_2D^+ ground-state transition are possible with APEX. In the future, ALMA observations of the resolved emission of H_2D^+ and other species will provide further insight into the chemical state of B68, and only with reliable collision rates will quantitative analysis of these observations be possible.

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